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DATE: Thursday, December 14, 2006

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<input type="checkbox"/>	L11	L10 and (site II or site 2 or site-2 or site-II)	1
<input type="checkbox"/>	L10	L9 and atomic coordinate	16
<input type="checkbox"/>	L9	glucocorticoid receptor and (crystal or x-ray)	725
		<i>DB=PGPB; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L8	17 and (site II or site 2 or site-2 or site-II)	1
<input type="checkbox"/>	L7	L6 and atomic coordinates	24
<input type="checkbox"/>	L6	glucocorticoid receptor and (crystal or x-ray)	877
		<i>DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L5	L1 and (three adj3 dimension\$3 structure or 3 adj2 D structure or crystal or x-ray)	26
<input type="checkbox"/>	L4	L1 and (three adj3 dimension\$3 structure or 3 adj2 D structure or crystal or x-ray)	26
		<i>DB=PGPB; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L3	L2 and (three adj3 dimension\$3 structure or 3 adj2 D structure or crystal or x-ray)	46
<input type="checkbox"/>	L2	Glucocorticoid receptor and (site II or site 2 or site-2 or site-II)	69
		<i>DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L1	Glucocorticoid receptor and (site II or site 2 or site-2 or site-II)	43

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As of Tuesday Dec 12, 2006 there are 40628 Structures | PDB Statistics

PDB ID or keyword Author **SEARCH** | Advanced Search

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☒ 1GDC

REFINED SOLUTION STRUCTURE OF THE GLUCOCORTICOID RECEPTOR DNA-BINDING DOMAIN

Release Date: 22-Jun-1994 Exp. Method: NMR

Characteristics
Classification
Glucocorticoid Receptor

Compound

Polymer: 1 Molecule: GLUCOCORTICOID RECEPTOR Chains: _

Authors

Baumann, H., Paulsen, K., Kovacs, H., Berglund, H., Wright, A.P., Gustafsson, J.A., Hard,

☒ 2GDA

REFINED SOLUTION STRUCTURE OF THE GLUCOCORTICOID RECEPTOR DNA-BINDING DOMAIN

Release Date: 22-Jun-1994 Exp. Method: NMR 24 Structures

Characteristics
Classification
Glucocorticoid Receptor

Compound

Polymer: 1 Molecule: GLUCOCORTICOID RECEPTOR Chains: _

Authors

Baumann, H., Paulsen, K., Kovacs, H., Berglund, H., Wright, A.P., Gustafsson, J.A., Hard,

☒ 1RGD

STRUCTURE REFINEMENT OF THE GLUCOCORTICOID RECEPTOR-DNA BINDING DOMAIN FROM NMR DATA BY RELAXATION MATRIX CALCULATIONS

Release Date: 14-Feb-1995 Exp. Method: NMR 11 Structures

Characteristics
Classification
DNA Binding Protein

Compound

Polymer: 1 Molecule: GLUCOCORTICOID RECEPTOR Chains: _

van Tilborg, M.A., Bonvin, A.M., Hard, K., Davis, A.L., Maler, B., Boelens, R., Yamamoto, K.R., Kaptein, R.

☒ 1R4R

Crystallographic analysis of the interaction of the glucocorticoid receptor with DNA



Characteristics
Release Date: 28-Oct-2003 Exp. Method: X Ray Diffraction
Resolution: 3.00 Å

Classification
Transcription/dna

Compound
Polymer: 1 Molecule: 5'-D(*TP*CP*AP*GP*AP*CP*AP*TP*GP*AP*TP*GP*TP*CP*TP*CP*
3' Chains: C Other Details: Idealized glucocorticoid response element IR3, top strand
Polymer: 2 Molecule: 5'-D(*CP*TP*GP*AP*GP*AP*CP*AP*TP*CP*AP*TP*GP*TP*CP*TP*
3' Chains: D Other Details: Idealized glucocorticoid response element IR3, bottom strand
Polymer: 3 Molecule: Glucocorticoid receptor Fragment: DNA binding domain Chains: A,B

Authors
Luisi, B.F., Xu, W.X., Otwinowski, Z., Freedman, L.P., Yamamoto, K.R., Sigler, P.B.

1R40



Crystallographic analysis of the interaction of the glucocorticoid receptor with DNA

Characteristics
Release Date: 21-Oct-2003 Exp. Method: X Ray Diffraction

Resolution: 2.50 Å

Classification
Transcription/dna



Compound
Polymer: 1 Molecule: 5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*CP*TP*
3' Chains: C,D

Authors
Polymer: 2 Molecule: Glucocorticoid receptor Fragment: DNA binding domain Chains: A,B
Luisi, B.F., Xu, W.X., Otwinowski, Z., Freedman, L.P., Yamamoto, K.R., Sigler, P.B.

1GLU



CRYSTALLOGRAPHIC ANALYSIS OF THE INTERACTION OF THE GLUCOCORTICOID RECEPTOR WITH DNA

Characteristics
Release Date: 31-Jan-1994 Exp. Method: X Ray Diffraction

Resolution: 2.90 Å

Classification
Transcription/dna



Compound
Polymer: 1 Molecule: DNA (5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*TP*CP*GP*AP*TP*GP*TP*CP*
P*TP*G-3') Chains: C,D

Authors
Polymer: 2 Molecule: PROTEIN (GLUCOCORTICOID RECEPTOR) Chains: A,B
Luisi, B.F., Xu, W.X., Otwinowski, Z., Freedman, L.P., Yamamoto, K.R., Sigler, P.B.

1WXX



Solution structure of the ubiquitin domain of BCL-2 binding athanogene-1

Characteristics
Release Date: 02-Aug-2005 Exp. Method: NMR 2D Structures

Classification
Apoptosis

Compound
Polymer: 1 Molecule: BAG-family molecular chaperone regulator-1 Fragment: ubiquitin-like domain
Chains: A



Authors

Niraula, T.N., Muto, Y., Inoue, M., Kigawa, T., Yokoyama, S.

☒ 1L2I

Human Estrogen Receptor alpha Ligand-binding Domain in Complex with (R,R)-5,11-cis-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol and a Glucocorticoid Receptor Interacting Protein 1 NR box II Peptide

Release Date: 01-May-2002 Exp. Method: X Ray Diffraction

Resolution: 1.95 Å

Characteristics

Transcription Receptor/coactivator

Compound

Polymer: 1 Molecule: ESTROGEN RECEPTOR Fragment: ligand-binding domain (residues 297-55-
Chains: A,B

Polymer: 2 Molecule: GLUCOCORTICOID RECEPTOR-INTERACTING PROTEIN 1 Fragment: NR
box II (residues 686-698) Chains: C,D

Authors

Shiau, A.K., Barstad, D., Radek, J.T., Meyers, M.J., Nettles, K.W., Katzenellenbogen, B.S., Katzenellenbogen, J.A., Agard, D.A., Greene, G.L.

☒ 1WMO**Characteristics**

Release Date: 07-Sep-2004 Exp. Method: X Ray Diffraction

Resolution: 2.90 Å

Classification

Transcription/signaling Protein

Compound

Polymer: 1 Molecule: Peroxisome proliferator activated receptor gamma Fragment: residues 186-47
Chains: X

Polymer: 2 Molecule: 14-mer from Nuclear receptor coactivator 2 Chains: Y

Authors

Ostberg, T., Svensson, S., Selen, G., Uppenberg, J., Thor, M., Sundbom, M., Sydow-Backman, M., Gustavsson, A.L., Jendeborg, L.

☒ 1NHZ

Crystal Structure of the Antagonist Form of Glucocorticoid Receptor

Characteristics

Release Date: 06-May-2003 Exp. Method: X Ray Diffraction

Resolution: 2.30 Å

Classification

Hormone Receptor

Compound

Polymer: 1 Molecule: GLUCOCORTICOID RECEPTOR Fragment: residue 500-777, hinge and ster
binding domains Mutation: N517D, F602S, C638D Chains: A

Authors

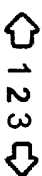
Kauppi, B., Jakob, C., Farnegardh, M., Yang, J., Ahola, H., Alarcon, M., Calles, K., Engstro O., Harlan, J., Muchmore, S., Ramqvist, A.-K., Thorell, S., Ohman, L., Greer, J., Gustafsson J.-A., Carlstedt-Duke, J., Carlquist, M.


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 PDB ID or keyword  Author   Advanced Search

26 Structure Hits 2 Unreleased Structures 126 Web Page Hits



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☒ 1LAT



GLUCOCORTICOID RECEPTOR MUTANT/DNA COMPLEX

Characteristics

Release Date: 18-Dec-1995 Exp. Method: X Ray Diffraction

Classification

Resolution: 1.90 Å

Compound

Transcription/dna

Authors

Authors

Polymer: 1 Molecule: DNA (5-D(*TP*TP*CP*CP*AP*GP*AP*AP*CP*AP*TP*GP*TP*CP*TP*GP*GP*A)-3) Chains: C,D
Polymer: 2 Molecule: PROTEIN (GLUCOCORTICOID RECEPTOR) Chains: A,B
Gewirth, D.T., Sigler, P.B.

☒ 1OSV



STRUCTURAL BASIS FOR BILE ACID BINDING AND ACTIVATION OF THE NUCLEAR RECEPTOR FXR

Characteristics

Release Date: 23-Mar-2004 Exp. Method: X Ray Diffraction

Classification

Resolution: 2.50 Å

Compound

DNA Binding Protein

Authors

Polymer: 1 Molecule: Bile acid receptor Fragment: ligand binding domain (FXR-LBD) Chains: A,B
Polymer: 2 Molecule: Nuclear receptor coactivator 2 Fragment: Residues (741-752) Chains: C,D,E
Mi, L.Z., Devarakonda, S., Harp, J.M., Han, Q., Pellicciari, R., Willson, T.M., Khorasanizadeh, S., Rastinejad, F.

☒ 1M2Z



Crystal structure of a dimer complex of the human glucocorticoid receptor ligand-binding domain bound to dexamethasone and a TIF2 coactivator motif

Characteristics

Release Date: 15-Jul-2003 Exp. Method: X Ray Diffraction

Classification

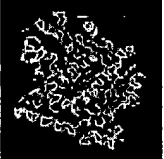


Resolution: 2.50 Å

Compound

Hormone/hormone Activator

Authors

Polymer: 1 Molecule: glucocorticoid receptor Fragment: Ligand Binding Domain, residues 521-777
Mutation: F602S Chains: A,D

3ERD   
 Polymer: 2 Molecule: nuclear receptor coactivator 2 Fragment: TIF2 coactivator motif, residues 734-754 Chains: B,E
 Bledsoe, R.B., Montana, V.G., Stanley, T.B., Delves, C.J., Apolito, C.J., McKee, D.D., Conshi T.G., Parks, D.J., Stewart, E.L., Willison, T.M., Lambert, M.H., Moore, J.T., Pearce, K.H., Xi H.E.



HUMAN ESTROGEN RECEPTOR ALPHA LIGAND-BINDING DOMAIN IN COMPLEX WITH DIETHYLSTILBESTROL AND A GLUCOCORTICOID RECEPTOR INTERACTING PROTEIN 1 NR BOX II PEPTIDE

Release Date: 08-Apr-1999 Exp. Method: X Ray Diffraction

Resolution: 2.03 Å

Nuclear Receptor

Compound 
 Polymer: 1 Molecule: PROTEIN (ESTROGEN RECEPTOR ALPHA) Fragment: LIGAND-BINDING DOMAIN Chains: A,B

Authors  
 Polymer: 2 Molecule: PROTEIN (GLUCOCORTICOID RECEPTOR INTERACTING PROTEIN 1) Fragment: NUCLEAR RECEPTOR BOX II Chains: C,D


Shiau, A.K., Barstad, D., Loria, P.M., Cheng, L., Kushner, P.J., Agard, D.A., Greene, G.L.

Human estrogen receptor alpha ligand-binding domain and a glucocorticoid receptor-interacting protein 1 NR box II peptide

Release Date: 19-Sep-2006 Exp. Method: X Ray Diffraction

Resolution: 2.10 Å

Hormone/growth Factor Receptor

Compound 
 Polymer: 1 Molecule: Estrogen receptor Fragment: LIGAND BINDING DOMAIN Mutation: S537Y Chains: A,B

Authors  
 Polymer: 2 Molecule: Nuclear receptor coactivator 2 Fragment: RESIDUES 686 - 698 Chains: C,D

Hsieh, R.W., Greene, G.L.



CRYSTAL STRUCTURE OF THE AGONIST FORM OF GLUCOCORTICOID RECEPTOR

Release Date: 08-Jul-2003 Exp. Method: X Ray Diffraction

Resolution: 2.70 Å

Hormone Receptor

Compound 
 Polymer: 1 Molecule: Glucocorticoid receptor Fragment: RESIDUE 500-777, hinge and steroid bind domains Mutation: N517D, F602S, C638D Chains: A,B,C,D

Authors  
 Polymer: 2 Molecule: Nuclear receptor coactivator 2 Fragment: TIF PEPTIDE 12mer Chains: E,F,G
 Kauppi, B., Jakob, C., Farnegardh, M., Yang, J., Ahola, H., Alarcon, M., Calles, K., Engstro O., Harlan, J., Muchmore, S., Ramqvist, A.-K., Thorell, S., Ohman, L., Greer, J., Gustafsson

J.-A. Carlstedt-Duke, J., Carlquist, M.

☒ 1UOM



THE STRUCTURE OF ESTROGEN RECEPTOR IN COMPLEX WITH A SELECTIVE AND POTENT TETRAHYDROISOCHOLIN LIGAND.

Characteristics

Release Date: 03-Jul-2003 Exp. Method: X Ray Diffraction

Classification

Resolution: 2.28 Å

Compound

Nuclear Protein

Authors

Polymer: 1 Molecule: ESTROGEN RECEPTOR Fragment: LIGAND BINDING DOMAIN, RESIDUE: 301 - 553 Mutation: YES Chains: A Other Details: NVP-ADD562 L SOLVENT S Renaud, J., Bischoff, S.F., Buhl, T., Floersheim, P., Fournier, B., Halleux, C., Kallen, J., Keller, H., Schiaepi, J.-M., Stark, W.

☒ 1GS4



STRUCTURAL BASIS FOR THE GLUCOCORTICOID RESPONSE IN A MUTANT HUMAN ANDROGEN RECEPTOR (ARCCR) DERIVED FROM AN ANDROGEN-INDEPENDENT PROSTATE CANCER

Characteristics

Release Date: 16-Jan-2003 Exp. Method: X Ray Diffraction

Classification

Resolution: 1.95 Å

Compound

Androgen Receptor

Authors

Polymer: 1 Molecule: ANDROGEN RECEPTOR Fragment: LIGAND-BINDING DOMAIN, RESIDUE 670-917 Mutation: YES Chains: A Matias, P.M., Carrondo, M.A., Coelho, R., Thomaz, M., Zhao, X., Wegg, A., Crusius, K., Egner, U., Donner, P.

☒ 1L2J



Human Estrogen Receptor beta Ligand-binding Domain In Complex with (R,R)-5,11-cis-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol

Characteristics

Release Date: 01-May-2002 Exp. Method: X Ray Diffraction

Classification

Resolution: 2.95 Å

Compound

Transcription Receptor

Authors

Polymer: 1 Molecule: ESTROGEN RECEPTOR BETA Fragment: ligand-binding domain (residues 256-505) Chains: A,B Shiau, A.K., Barstad, D., Radek, J.T., Meyers, M.J., Nettles, K.W., Katzenellenbogen, B.S., Katzenellenbogen, J.A., Agard, D.A., Greene, G.L.

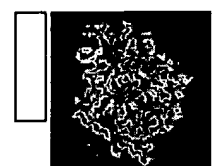
☒ 2B1V



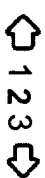
Human estrogen receptor alpha ligand-binding domain in complex with OBCP-1M and a glucocorticoid receptor interacting protein 1 NR box II peptide

Characteristics

Release Date: 09-May-2006 Exp. Method: X Ray Diffraction






Classification	Resolution: 1.80 Å
Compound	Hormone/growth Factor Receptor
Authors	Polymer: 1 Molecule: Estrogen receptor Fragment: LIGAND BINDING DOMAIN Mutation: Y537S Chains: A,B Polymer: 2 Molecule: Nuclear receptor coactivator 2 Fragment: RESIDUES 686 - 698 Chains: C,D Hsieh, R.W., Rajan, S.S., Sharma, S.K., Guo, Y., Desombre, E.R., Mrksich, M., Greene, G.L.



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☒ 2BJ4



ESTROGEN RECEPTOR ALPHA LBD IN COMPLEX WITH A PHAGE-DISPLAY DERIVED PEPTIDE ANTAGONIST

Release Date: 16-Feb-2005 Exp. Method: X Ray Diffraction

Resolution: 2.00 Å

Nuclear Receptor

Compound

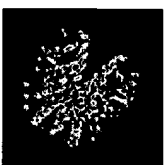
Polymer: 1 Molecule: ESTROGEN RECEPTOR Fragment: RESIDUES 305-533 (LIGAND-BINDING DOMAIN) Chains: A,B

Polymer: 2 Molecule: PEPTIDE ANTAGONIST Chains: C,D

Authors

Kong, E., Heldring, N., Gustafsson, J.A., Treuter, E., Hubbard, R.E., Pike, A.C.W.

☒ 1QKT



MUTANT ESTROGEN NUCLEAR RECEPTOR LIGAND BINDING DOMAIN COMPLEXED WITH ESTRADIOL

Release Date: 18-Aug-2000 Exp. Method: X Ray Diffraction

Resolution: 2.20 Å

Nuclear Receptor

Compound

Polymer: 1 Molecule: ESTRADIOL RECEPTOR Fragment: LIGAND BINDING DOMAIN

Mutation: YES Chains: A

Authors

Gangloff, M., Ruff, M., Eiler, S., Duclaud, S., Wurtz, J.M., Moras, D.

☒ 1ZKY



Human Estrogen Receptor Alpha Ligand-Binding Domain In Complex With OBCP-3M and A Glucocorticoid Receptor Interacting Protein 1 Nr Box II Peptide

Release Date: 09-May-2006 Exp. Method: X Ray Diffraction

Resolution: 2.25 Å

Hormone/growth Factor Receptor

Compound

Polymer: 1 Molecule: Estrogen receptor Fragment: Ligand Binding Domain Mutation: Y537S

Chains: A,B

Polymer: 2 Molecule: Nuclear receptor coactivator 2 Fragment: Residues 686 - 698 Chains: C,D

Authors

Hsieh, R.W., Rajan, S.S., Sharma, S.K., Guo, Y., Desombre, E.R., Mrksich, M., Greene, G.L.

☒ 2FAI**Human Estrogen Receptor Alpha Ligand-Binding Domain In Complex With OBCP-2M and A Glucocorticoid Receptor Interacting Protein 1 NR Box II Peptide****Characteristics**

Release Date: 09-May-2006 Exp. Method: X Ray Diffraction

Resolution: 2.10 Å

Classification**Hormone/growth Factor Receptor****Compound**

Polymer: 1 Molecule: Estrogen receptor Fragment: LIGAND BINDING DOMAIN Chains: A,B

Polymer: 2 Molecule: Nuclear receptor coactivator 2 Chains: C,D

Authors

Hsieh, R.W., Rajan, S.S., Sharma, S.K., Guo, Y., Desombre, E.R., Mrksich, M., Greene, G.L.

☒ 1QKU**WILD TYPE ESTROGEN NUCLEAR RECEPTOR LIGAND BINDING DOMAIN COMPLEXED WITH ESTRADIOL****Characteristics**

Release Date: 18-Aug-2000 Exp. Method: X Ray Diffraction

Resolution: 3.20 Å

Classification**Nuclear Receptor****Compound**

Polymer: 1 Molecule: ESTRADIOL RECEPTOR Fragment: LIGAND BINDING DOMAIN

Chains: A,B,C

Authors

Ruff, M., Gangloff, M., Eiler, S., Duclaud, S., Wurtz, J.M., Dino, M.

☒ 1HX1**CRYSTAL STRUCTURE OF A BAG DOMAIN IN COMPLEX WITH THE HSC70 ATPASE DOMAIN****Characteristics**

Release Date: 07-Mar-2001 Exp. Method: X Ray Diffraction

Resolution: 1.90 Å

Classification**Chaperone/chaperone Inhibitor****Compound**

Polymer: 1 Molecule: HEAT SHOCK COGNATE 71 KDA Fragment: ATPASE DOMAIN Chains: A

Polymer: 2 Molecule: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1 Fragment: BAG

DOMAIN Chains: B

Authors

Sondermann, H., Scheuffer, C., Schneider, C., Hohfeld, J., Hartl, F.U., Moarefi, I.

1 2 3

STN Search

10/621,807

FILE 'HOME' ENTERED AT 17:44:50 ON 14 DEC 2006

=> file .nash

=> s glucocorticoid receptor and (three (5w) structure or 3(1w)D structure or model or crystal)

L1 1091 FILE MEDLINE
L2 1007 FILE CAPLUS
L3 1385 FILE SCISEARCH
L4 274 FILE LIFESCI
L5 1171 FILE BIOSIS
L6 1596 FILE EMBASE

TOTAL FOR ALL FILES

L7 6524 GLUCOCORTICOID RECEPTOR AND (THREE (5W) STRUCTURE OR 3(1W) D
STRUCTURE OR MODEL OR CRYSTAL)

=> s glucocorticoid receptor and (three (1w) dimension? structure or 3(1w)D structure)

TOTAL FOR ALL FILES

L14 101 GLUCOCORTICOID RECEPTOR AND (THREE (1W) DIMENSION? STRUCTURE OR
3(1W) D STRUCTURE)

=> dup rem l14

PROCESSING COMPLETED FOR L14

L29 34 DUP REM L14 (67 DUPLICATES REMOVED)

=> s l29 not 2003-2006/py

TOTAL FOR ALL FILES

L42 24 L29 NOT 2003-2006/PY

=> d ibib abs 1-24

L42 ANSWER 1 OF 24 MEDLINE on STN

ACCESSION NUMBER: 2002396367 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12144349

TITLE: Homology modelling of the ligand binding domain of
mineralocorticoid receptor: close structural kinship with
glucocorticoid receptor ligand binding
domain and their similar binding mode with DOC (de-oxy
corticosterone).

AUTHOR: Dey Raja; Roychowdhury P

CORPORATE SOURCE: Dept. of Physics, University of Calcutta, 92 A.P.C. Road,
India.SOURCE: Journal of biomolecular structure & dynamics, (2002 Aug)
Vol. 20, No. 1, pp. 21-9.

Journal code: 8404176. ISSN: 0739-1102.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200302

ENTRY DATE: Entered STN: 30 Jul 2002

Last Updated on STN: 27 Feb 2003

Entered Medline: 26 Feb 2003

AB Mineralocorticoids play a major role in regulating sodium and potassium homeostasis and also contribute to the control of blood pressure and in some physiological disorders. The physiological effects of this class of corticosteroids are mediated by ligand-induced nuclear transcription factor, the mineralocorticoid receptor(MR) / glucocorticoid receptor(GR), a member of the steroid / nuclear receptor superfamily. Although the MR interacts with both glucocorticoids and mineralocorticoids, the GR interacts specifically with glucocorticoids. The three dimensional structure of progesterone complexed to its receptor revealed in X-ray diffraction method is utilised to develop a homology model of human mineralocorticoid receptor ligand binding domain (hMR LBD) in a similar fashion as mouse GR LBD was developed previously. The secondary structure of hMR LBD contains eleven helices, eight turns and four sheets. This receptor contains a long helix, H9, with thirty four residues. The 12-residue C-terminal extension (residues 973-984) of hMR LBD, which is essential for hormone binding, is tightly fixed in position by an antiparallel b-sheet interaction. The three dimensional model reveals two polar sites located at the extremities of the elongated hydrophobic ligand-binding pocket (LBP). De-oxy corticosterone (DOC) is docked to the LBs of both hMR LBD and mGR LBD. The difference accessible surface area (DASA) study revealed the interaction zones of both the receptors in complex with DOC. Observations relating to the native and complex proteins revealed a close structural kinship between hMR LBD and mGR LBD.

L42 ANSWER 2 OF 24 MEDLINE on STN

ACCESSION NUMBER: 2000438446 MEDLINE Full-text
 DOCUMENT NUMBER: PubMed ID: 10966797
 TITLE: Mutations in the glucocorticoid receptor
 DNA-binding domain mimic an allosteric effect of DNA.
 AUTHOR: van Tilborg M A; Lefstin J A; Kruiskamp M; Teuben J;
 Boelens R; Yamamoto K R; Kaptein R
 CORPORATE SOURCE: Bijvoet Center for Biomolecular Research, Padualaan 8,
 Utrecht, NL3584CH, The Netherlands.
 SOURCE: Journal of molecular biology, (2000 Aug 25) Vol. 301, No.
 4, pp. 947-58.
 Journal code: 2985088R. ISSN: 0022-2836.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200009
 ENTRY DATE: Entered STN: 28 Sep 2000
 Last Updated on STN: 28 Sep 2000
 Entered Medline: 21 Sep 2000

AB Two previously isolated mutations in the glucocorticoid receptor DNA-binding domain (DBD), S459A and P493R, have been postulated to mimic DNA-induced conformational changes in the glucocorticoid receptor DBD, thereby constitutively triggering an allosteric mechanism in which binding of specific DNA normally induces the exposure of otherwise silent glucocorticoid receptor transcriptional activation surfaces. Here we report the three-dimensional structure of the free S459A and P493R mutant DBDs as determined by NMR spectroscopy. The free S459A and P493R structures both display the conformational changes in the DBD dimerization interface that are characteristic of the DNA-bound wild-type DBD, confirming that these mutations mimic an allosteric effect of DNA. A transition between two packing arrangements of the DBD hydrophobic core provides a mechanism for long-range transmission of conformational changes, induced either by the mutations or by DNA binding, to protein-protein contact surfaces.
 Copyright 2000 Academic Press.

L42 ANSWER 3 OF 24 MEDLINE on STN
 ACCESSION NUMBER: 1999333138 MEDLINE Full-text
 DOCUMENT NUMBER: PubMed ID: 10406480
 TITLE: The structure of the nuclear hormone receptors.
 AUTHOR: Kumar R; Thompson E B
 CORPORATE SOURCE: Department of Human Biological Chemistry and Genetics,
 University of Texas Medical Branch at Galveston,
 77555-0645, USA.
 SOURCE: Steroids, (1999 May) Vol. 64, No. 5, pp. 310-9. Ref: 80
 Journal code: 0404536. ISSN: 0039-128X.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 General Review; (REVIEW)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199909
 ENTRY DATE: Entered STN: 25 Sep 1999
 Last Updated on STN: 25 Sep 1999
 Entered Medline: 16 Sep 1999

AB The functions of the group of proteins known as nuclear receptors will be understood fully only when their working three-dimensional structures are known. These ligand-activated transcription factors belong to the steroid-thyroid-retinoid receptor superfamily, which include the receptors for steroids, thyroid hormone, vitamins A- and D-derived hormones, and certain fatty acids. The majority of family members are homologous proteins for which no ligand has been identified (the orphan receptors). Molecular cloning and structure/function analyses have revealed that the members of the superfamily have a common functional domain structure. This includes a variable N-terminal domain, often important for transactivation of transcription; a well conserved DNA-binding domain, crucial for recognition of specific DNA sequences and protein:protein interactions; and at the C-terminal end, a ligand-binding domain, important for hormone binding, protein:protein interactions, and additional transactivation activity. Although the structure of some independently expressed single domains of a few of these receptors have been solved, no holoreceptor structure or structure of any two domains together is yet available. Thus, the three-dimensional structure of the DNA-binding domains of the glucocorticoid, estrogen, retinoic acid-beta, and retinoid X receptors, and of the ligand-binding domains of the thyroid, retinoic acid-gamma, retinoid X, estrogen, progesterone, and peroxisome proliferator activated-gamma receptors have been solved. The secondary structure of the glucocorticoid receptor N-terminal domain, in particular the transcription activation region, has also been studied. The structural studies available not only provide a beginning stereochemical knowledge of these receptors, but also a basis for understanding some of the topological details of the interaction of the receptor complexes with coactivators, corepressors, and other components of the transcriptional machinery. In this review, we summarize and discuss the current information on structures of the steroid-thyroid-retinoid receptors.

L42 ANSWER 4 OF 24 MEDLINE on STN

ACCESSION NUMBER: 97047406 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 9121489

TITLE: Mutation of isoleucine 747 by a threonine alters the ligand responsiveness of the human glucocorticoid receptor.

AUTHOR: Roux S; Terouanne B; Balaguer P; Jausons-Loffreda N; Pons M; Chambon P; Gronemeyer H; Nicolas J C

CORPORATE SOURCE: INSERM U439, Montpellier, France.

SOURCE: Molecular endocrinology (Baltimore, Md.), (1996 Oct) Vol. 10, No. 10, pp. 1214-26.

Journal code: 8801431. ISSN: 0888-8809.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199704

ENTRY DATE: Entered STN: 6 May 1997

Last Updated on STN: 6 May 1997

Entered Medline: 23 Apr 1997

AB Mutation of isoleucine 747 to threonine in the C-terminal part of the ligand-binding domain (LBD) of the human glucocorticoid receptor (GR) alters the ligand specificity for transactivation. Natural glucocorticoids such as cortisol or corticosterone were completely inactive with the mutant 1747T, whereas synthetic steroids like dexamethasone efficiently stimulated GR 1747T-mediated transactivation. However, the corresponding ligand dose-response curve for dexamethasone-induced transactivation was shifted to higher concentrations when compared with that obtained with the wild type GR. Neither this shift nor the inability of cortisol to activate the 1747T mutant was due to an altered in vitro ligand-binding affinity. In the canonical three-dimensional structure of nuclear receptor LBDs, isoleucine 747 is in the direct vicinity of residues that contribute to the ligand-binding pocket. Moreover, it is located in the C-terminal LBD region, which harbors the conserved core of the activation function AF-2 and undergoes a ligand-induced transconformation, required to generate the surface interacting with putative transcriptional intermediary factors/coactivators of AF-2. The phenotype of 1747T mutant is discussed in view of the possible consequences of the mutation on the various events which, according to the model, lead to a transcriptionally competent AF-2.

L42 ANSWER 5 OF 24 MEDLINE on STN

ACCESSION NUMBER: 96133733 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 8548460

TITLE: A canonical structure for the ligand-binding domain of nuclear receptors.

AUTHOR: Wurtz J M; Bourguet W; Renaud J P; Vivat V; Chambon P; Moras D; Gronemeyer H

CORPORATE SOURCE: Institut de Genetique et de Biologie Moleculaire et Cellulaire, CNRS/INSERM/ULP/C, College de France, Illkrich, C.U. de Strasbourg, France.

SOURCE: Nature structural biology, (1996 Jan) Vol. 3, No. 1, pp. 87-94.

Journal code: 9421566. ISSN: 1072-8368.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199602

ENTRY DATE: Entered STN: 6 Mar 1996

Last Updated on STN: 19 Jul 1996

Entered Medline: 21 Feb 1996

AB The ability of nuclear receptors (NRs) to activate transcription of target genes requires the binding of cognate ligands to their ligand-binding domains (LBDs). Information provided by the three-dimensional structures of the unliganded RXR alpha and the liganded RAR gamma LBDs has been incorporated into a general alignment of the LBDs of all NRs. A twenty amino-acid region constitutes a NR-specific signature and contains most of the conserved residues that stabilize the core of the canonical fold of NR LBDs. A common ligand-binding pocket, involving predominantly hydrophobic residues, is inferred by homology modelling of the human RXR alpha and glucocorticoid receptor ligand-binding sites according to the RAR gamma holo-LBD structure. Mutant studies support these models, as well as a general mechanism for ligand-induced activation deduced from the comparison of the transcriptionally active RAR gamma holo- and inactive RXR alpha apo-LBD structures.

L42 ANSWER 6 OF 24 MEDLINE on STN

ACCESSION NUMBER: 95087885 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 7995522
 TITLE: Influence of a steroid receptor DNA-binding domain on transcriptional regulatory functions.
 AUTHOR: Lefstin J A; Thomas J R; Yamamoto K R
 CORPORATE SOURCE: Department of Pharmacology, University of California at San Francisco 94143-0450.
 SOURCE: Genes & development, (1994 Dec 1) Vol. 8, No. 23, pp. 2842-56.
 Journal code: 8711660. ISSN: 0890-9369.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199501
 ENTRY DATE: Entered STN: 26 Jan 1995
 Last Updated on STN: 3 Feb 1997
 Entered Medline: 17 Jan 1995

AB We have isolated two independent mutations in the DNA-binding domain of the rat glucocorticoid receptor, P493R and S459A, that implicate DNA binding in the control of attached transcriptional activation domains, either that of the receptor itself or of VP16. The mutants are capable of activating transcription normally, but unlike wild-type receptors, they interfere with particular transcriptional activators in yeast and mammalian cells, and inhibit growth when overexpressed in yeast. The mutant residues reside at positions within the three-dimensional structure of the receptor that could, in principle, transduce structural changes from the DNA-binding surface of the receptor to other functional domains. These findings, together with the salt dependence of specific and nonspecific DNA binding by these receptors, suggest that specific DNA acts as an allosteric effector that directs the functional interaction of the receptor with targets of transcriptional activation and that the P493R and S459A mutants mimic the allosteric effect of specific DNA, allowing the receptor to interact with regulatory targets even in the absence of specific DNA binding.

L42 ANSWER 7 OF 24 MEDLINE on STN
 ACCESSION NUMBER: 94185649 MEDLINE Full-text
 DOCUMENT NUMBER: PubMed ID: 8137826
 TITLE: The dimerization interfaces formed between the DNA binding domains of RXR, RAR and TR determine the binding specificity and polarity of the full-length receptors to direct repeats.
 AUTHOR: Zechel C; Shen X Q; Chen J Y; Chen Z P; Chambon P; Gronemeyer H
 CORPORATE SOURCE: Laboratoire de Genetique Moleculaire des Eucaryotes du CNRS et Unite 184 de Biologie Moleculaire et de Genie Genetique de l'INSERM, Faculte de Medecine, Strasbourg, France.
 SOURCE: The EMBO journal, (1994 Mar 15) Vol. 13, No. 6, pp. 1425-33.
 Journal code: 8208664. ISSN: 0261-4189.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199404
 ENTRY DATE: Entered STN: 9 May 1994
 Last Updated on STN: 9 May 1994
 Entered Medline: 22 Apr 1994

AB Heterodimers of retinoid X receptor (RXR) and retinoic acid receptor (RAR) bind preferentially to directly repeated elements with spacing of two (DR2) or five (DR5) base pairs, due to the specific heterocooperative interaction of their DNA binding domains (DBDs) on these elements. We have demonstrated in the accompanying paper that the heterodimeric DBD interface that is responsible for the cooperative binding to DR5 elements, specifically involves the D-box of the RXR CII finger and the tip of the RAR CI finger. We show here that a second type of dimerization interface, which specifically implicates the RAR T-box and the RXR CII finger to the exclusion of the D-box, determines the selective binding to DR2 elements. Interestingly, the same type of dimerization interface (RXR T-box and CII finger) is responsible for the cooperative binding of homodimers of the RXR DBD to DR1 elements. Based on the three-dimensional structure of the glucocorticoid receptor DBD, modeling of RXR/RAR, RXR/TR and RXR/RXR DBD cooperative interactions predicts that in all cases the DBD contributing the CII finger, i.e. that of RXR, has to be positioned 5' to its cooperatively bound partner. This binding polarity of the DBDs is conferred upon the full-length receptors, since crosslinking experiments indicate that RXR is always 5' to RAR in complexes between either DR5 or DR2 and RXR/RAR heterodimers. The possible significance of these observations for transactivation by retinoic acid receptors is discussed.

L42 ANSWER 8 OF 24 MEDLINE on STN
 ACCESSION NUMBER: 93192652 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 8383553
 TITLE: The solution structure of the human retinoic acid receptor-beta DNA-binding domain.
 AUTHOR: Knegtel R M; Katahira M; Schilthuis J G; Bonvin A M; Boelens R; Eib D; van der Saag P T; Kaptein R
 CORPORATE SOURCE: Department of Chemistry, University of Utrecht, The Netherlands.
 SOURCE: Journal of biomolecular NMR, (1993 Jan) Vol. 3, No. 1, pp. 1-17.
 Journal code: 9110829. ISSN: 0925-2738.
 PUB. COUNTRY: Netherlands
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199304
 ENTRY DATE: Entered STN: 23 Apr 1993
 Last Updated on STN: 23 Apr 1993
 Entered Medline: 13 Apr 1993

AB The three-dimensional structure of the DNA-binding domain of the human retinoic acid receptor-beta (hRAR-beta) has been determined by nuclear magnetic resonance spectroscopy in conjunction with distance geometry, restrained molecular dynamics and iterative relaxation matrix calculations. A total of 1244 distance restraints were obtained from NOE intensities, of which 448 were intra-residue and 796 inter-residue restraints. In addition 23 chi and 30 phi dihedral angle restraints were obtained from J-coupling data. The two 'zinc-finger' regions of the 80-amino acid residue protein are followed by two alpha-helices that cross each other perpendicularly. There is a short stretch of b-sheet near the N-terminus. The alpha-helical core of the protein is well determined with a backbone root-mean-square deviation (r.m.s.d.) with respect to the average of 0.18 A and 0.37 A when the side chains of residues 31, 32, 36, 61, 62, 65 and 69 are included. The r.m.s.d. for the backbone of residues 5-80 is 0.76 A. For the first finger (residues 8-28), the r.m.s.d. of the backbone is 0.79 A. For the second finger (residues 44-62) the r.m.s.d. is 0.64 A. The overall structure is similar to that of the corresponding domain of the glucocorticoid receptor, although the C-terminal part of the protein is different. The second alpha-helix is two residues shorter and is followed by a well-defined region of extended backbone structure.

L42 ANSWER 9 OF 24 MEDLINE on STN
 ACCESSION NUMBER: 92222905 MEDLINE Full-text
 DOCUMENT NUMBER: PubMed ID: 1562506
 TITLE: DNA-binding by the glucocorticoid receptor: a structural and functional analysis.
 AUTHOR: Dahlman-Wright K; Wright A; Carlstedt-Duke J; Gustafsson J A
 CORPORATE SOURCE: Department of Medical Nutrition, Huddinge Hospital, Karolinska Institute, Sweden.
 SOURCE: The Journal of steroid biochemistry and molecular biology, (1992 Mar) Vol. 41, No. 3-8, pp. 249-72. Ref: 268
 Journal code: 9015483. ISSN: 0960-0760.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 General Review; (REVIEW)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199205
 ENTRY DATE: Entered STN: 7 Jun 1992
 Last Updated on STN: 7 Jun 1992
 Entered Medline: 18 May 1992

AB The glucocorticoid receptor belongs to a family of ligand activated nuclear receptors. This family includes, in addition to the receptors for steroid hormones, receptors for thyroid hormone, retinoic acid and 1,25-dihydroxy vitamin D3 as well as some receptors with as yet unknown ligands. The glucocorticoid receptor DNA-binding domain has been expressed in E. coli. The purified protein binds to the same DNA sequences as the native receptor and is therefore suitable for biochemical and structural studies of the DNA-binding function of the receptor protein. This protein has been shown to bind as a dimer to its DNA-binding site. Protein-protein interactions facilitate DNA-binding and a segment responsible for these interactions has been identified close to the C-terminal zinc-binding site. The family of nuclear receptors, with their related DNA-binding sites, provides an opportunity to study determinants for DNA sequence recognition. A segment close to the N-terminal zinc ion has been shown to be responsible for the target specificity of glucocorticoid and estrogen receptors. DNA-binding domains of nuclear receptors include nine conserved cysteine residues which have been shown to coordinate two zinc ions and zinc has been shown to be required for the structural integrity and DNA-binding ability of the glucocorticoid receptor DNA-binding domain. A motif for DNA recognition, based around zinc ions, was first described for transcription factor IIIA and nuclear receptors were believed to recognize DNA via a similar motif. However, the three-dimensional structure determination of the glucocorticoid receptor DNA-binding domain shows that its structure is clearly different from that of the TFIIIA type zinc-binding domains.

L42 ANSWER 10 OF 24 MEDLINE on STN

ACCESSION NUMBER: 92017877 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 1922092
TITLE: Identification of protein contact sites within the glucocorticoid/progestin response element.
AUTHOR: Cairns C; Gustafsson J A; Carlstedt-Duke J
CORPORATE SOURCE: Department of Medical Nutrition, Karolinska Institute, Huddinge University Hospital, Sweden.
SOURCE: Molecular endocrinology (Baltimore, Md.), (1991 Apr) Vol. 5, No. 4, pp. 598-604.
Journal code: 8801431. ISSN: 0888-8809.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199110
ENTRY DATE: Entered STN: 24 Jan 1992
Last Updated on STN: 24 Jan 1992
Entered Medline: 29 Oct 1991

AB The glucocorticoid receptor (GR) and the progestin receptor (PR) bind specifically to a variety of DNA sequences, glucocorticoid/progestin response elements (GRE/PRE), located in the proximity of responsive gene promoters. Using the isolated recombinant GR DNA-binding domain (DBD), it has recently been shown that GR interacts with the GRE/PRE, a 15-basepair partially palindromic consensus sequence, as a dimer. In this study an investigation into the GR-GRE/PRE and PR-GRE/PRE interaction has been performed using missing base contact analysis with the tyrosine aminotransferase GREII (TATII) and recombinant GR DBD as well as a fusion protein consisting of the PR DBD fused to Staph. aureus protein-A. GR and PR had identical base contact points, localized within two consecutive major grooves, binding to the same face of the DNA. Ethylation interference was also performed on the GR DBD-TATII interaction. The contact points with the backbone phosphate groups flank the contacts within the major groove for each of the two half-sites. Knowledge of the contact points within the DNA sequence together with the three-dimensional structure of the protein enables modelling of the protein-DNA interaction.

L42 ANSWER 11 OF 24 MEDLINE on STN

ACCESSION NUMBER: 91126121 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 1846973
TITLE: Zinc fingers, zinc clusters, and zinc twists in DNA-binding protein domains.
AUTHOR: Vallee B L; Coleman J E; Auld D S
CORPORATE SOURCE: Center for Biochemical and Biophysical Sciences and Medicine, Harvard Medical School, Brigham and Women's Hospital, Boston, MA 02115.
CONTRACT NUMBER: DK09070 (NIDDK)
GM21919 (NIGMS)
SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1991 Feb 1) Vol. 88, No. 3, pp. 999-1003.
Journal code: 7505876. ISSN: 0027-8424.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199103
ENTRY DATE: Entered STN: 5 Apr 1991
Last Updated on STN: 3 Feb 1997
Entered Medline: 8 Mar 1991

AB We now recognize three distinct motifs of DNA-binding zinc proteins: (i) zinc fingers, (ii) zinc clusters, and (iii) zinc twists. Until very recently, x-ray crystallographic or NMR three-dimensional structure analyses of DNA-binding zinc proteins have not been available to serve as standards of reference for the zinc binding sites of these families of proteins. Those of the DNA-binding domains of the fungal transcription factor GAL4 and the rat glucocorticoid receptor are the first to have been determined. Both proteins contain two zinc binding sites, and in both, cysteine residues are the sole zinc ligands. In GAL4, two zinc atoms are bound to six cysteine residues which form a "zinc cluster" akin to that of metallothionein; the distance between the two zinc atoms of GAL4 is approximately 3.5 Å. In the glucocorticoid receptor, each zinc atom is bound to four cysteine residues; the interatomic zinc-zinc distance is approximately 13 Å, and in this instance, a "zinc twist" is represented by a helical DNA recognition site located between the two zinc atoms. Zinc clusters and zinc twists are here recognized as two distinctive motifs in DNA-binding proteins containing multiple zinc atoms. For native "zinc fingers," structural data do not exist as yet; consequently, the interatomic distances between zinc atoms are not known. As further structural data become available, the structural and functional significance of these

different motifs in their binding to DNA and other proteins participating in the transmission of the genetic message will become apparent.

L42 ANSWER 12 OF 24 MEDLINE on STN

ACCESSION NUMBER: 90319784 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 2115209
TITLE: Solution structure of the glucocorticoid
receptor DNA-binding domain.
AUTHOR: Hard T; Kellenbach E; Boelens R; Maler B A; Dahlman K;
Freedman L P; Carlstedt-Duke J; Yamamoto K R; Gustafsson J
A; Kaptein R
CORPORATE SOURCE: Department of Chemistry, University of Utrecht, The
Netherlands.
SOURCE: Science, (1990 Jul 13) Vol. 249, No. 4965, pp. 157-60.
Journal code: 0404511. ISSN: 0036-8075.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199008
ENTRY DATE: Entered STN: 21 Sep 1990
Last Updated on STN: 3 Feb 1997
Entered Medline: 23 Aug 1990

AB The three-dimensional structure of the DNA-binding domain (DBD) of the glucocorticoid receptor has been determined by nuclear magnetic resonance spectroscopy and distance geometry. The structure of a 71-residue protein fragment containing two "zinc finger" domains is based on a large set of proton-proton distances derived from nuclear Overhauser enhancement spectra, hydrogen bonds in previously identified secondary structure elements, and coordination of two zinc atoms by conserved cysteine residues. The DBD is found to consist of a globular body from which the finger regions extend. A model of the dimeric complex between the DBD and the glucocorticoid response element is proposed. The model is consistent with previous results indicating that specific amino acid residues of the DBD are involved in protein-DNA and protein-protein interactions.

L42 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:428305 CAPLUS Full-text
DOCUMENT NUMBER: 134:361467
TITLE: New development of steroid
AUTHOR(S): Tanaka, Hirotooshi
CORPORATE SOURCE: The Inst. Med. Sci., The Univ. Tokyo, Japan
SOURCE: Ensho to Men'eki (2001), 9(3), 353-360
CODEN: ENMEFA; ISSN: 0918-8371
PUBLISHER: Sentan Igakusha
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

AB A review with 45 refs., on the physiol. functions of glucocorticoids, domain structure and three-dimensional structure of glucocorticoid receptor (GR), transcriptional regulation by GR, interactions between GR and AP-1 and between GR and NF- κ B, redox regulation of GR functions, development of novel GR ligands for antiinflammatory agents or immunosuppressants, and future prospect of steroid therapy.

L42 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:57327 CAPLUS Full-text
DOCUMENT NUMBER: 132:189750
TITLE: Structure and functions of nuclear hormone receptors
AUTHOR(S): Kumar, R.; Srinivasan, G.; Thompson, E. B.
CORPORATE SOURCE: Department of Human Biological Chemistry and Genetics,
University of Texas Medical Branch, Galveston, TX,
77555-0645, USA
SOURCE: Current Topics in Steroid Research (1998), 1, 19-35
CODEN: CTSRFV
PUBLISHER: Research Trends
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review, with 165 refs., on the nuclear hormone receptor superfamily. This superfamily includes receptors for steroids, thyroid hormone, vitamin A, and D derived hormones, and certain fatty acids, as well as transcription factors for which no ligand has been identified (the so called orphan receptors). All family members are intracellular transcription factors, and the true receptors mediate the biol. effects of their resp. hormones, primarily at the level of gene regulation, by binding to specific DNA sequences known as hormone response element (HRE) and by protein:protein interaction with other transcription factors. Each receptor protein is organized into several major functional domains. The major domains are those important for transactivation, site-specific DNA binding and ligand binding. The DNA binding domain (DBD), which is the most

conserved region among this entire superfamily, is responsible for receptors' ability to discriminate between their specific response element and other DNA sequences. The ligand binding domain (LBD) is responsible for discriminating between various ligands and is also the site for interaction with certain other proteins. Transactivation domains may be found in the N-terminal region and/or within the LBD, depending on the particular receptor. The structure of some domains of a few of this receptor family have been solved. The three dimensional structure of the DBDs of the glucocorticoid, estrogen and retinoid X receptors, and of the LBD of the thyroid receptor with thyroid hormone bound, the retinoic acid receptor- γ with all -trans retinoic acid bound, as well as the unliganded retinoid X and estrogen receptors have been solved. The secondary structure of the taut transcription activation region in the N-terminal domain of the glucocorticoid receptor has also been demonstrated. No complete structure or the structure of any two domains together is yet available for proteins of this family.

REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 15 OF 24 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1999:72541 SCISEARCH Full-text

THE GENUINE ARTICLE: 158JR

TITLE: Investigation of the binding interactions of progesterone using muteins of the human progesterone receptor ligand binding domain designed on the basis of a three-dimensional protein model

AUTHOR: Letz M; Bringmann P; Mann M; Mueller-Fahrnow A; Reipert D; Scholz P; Wurtz J M; Egner U (Reprint)

CORPORATE SOURCE: Schering AG, Res Labs, D-13342 Berlin, Germany (Reprint); Struct Biol Lab, IGBMC, F-67404 Illkirch Graffenstaden, France

COUNTRY OF AUTHOR: Germany; France

SOURCE: BIOCHIMICA ET BIOPHYSICA ACTA-PROTEIN STRUCTURE AND MOLECULAR ENZYMOLOGY, (11 JAN 1999) Vol. 1429, No. 2, pp. 391-400.

ISSN: 0167-4838.

PUBLISHER: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS.

DOCUMENT TYPE: Article; Journal

LANGUAGE: English

REFERENCE COUNT: 28

ENTRY DATE: Entered STN: 1999

Last Updated on STN: 1999

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The aim of this study was to investigate the binding interactions of the human progesterone receptor (hPR) with its natural ligand. Therefore, a homology-derived model of the hPR ligand binding domain has been constructed and used to predict residues potentially involved in interactions with progesterone. These residues and the free cysteines have been mutated (in total 13 residues with 15 mutations). All exchanges have been designed to preserve the three-dimensional structure of the protein. With respect to the binding characteristics towards progesterone, the muteins fall into three groups displaying no, reduced, or wildtype-like binding activity. (C) 1999 Elsevier Science B.V. All rights reserved.

L42 ANSWER 16 OF 24 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1993:530267 SCISEARCH Full-text

THE GENUINE ARTICLE: LU404

TITLE: PROTEIN NUCLEIC-ACID INTERACTIONS BY NMR

AUTHOR: KAPTEIN R

CORPORATE SOURCE: UNIV UTRECHT, UTRECHT, NETHERLANDS

COUNTRY OF AUTHOR: NETHERLANDS

SOURCE: CURRENT OPINION IN STRUCTURAL BIOLOGY, (FEB 1993) Vol. 3, No. 1, pp. 50-56.

ISSN: 0959-440X.

PUBLISHER: CURRENT BIOLOGY LTD, 34-42 CLEVELAND STREET, LONDON, ENGLAND W1P 6LB.

DOCUMENT TYPE: Article; Journal

LANGUAGE: English

REFERENCE COUNT: 47

ENTRY DATE: Entered STN: 1994

Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB NMR spectroscopy has been remarkably successful as a tool for elucidating the three-dimensional structures of DNA-binding proteins. Several DNA-binding domains of bacterial repressors and eukaryotic transcription factors, together with, in some cases, their complexes with DNA, have been analyzed by NMR. Highlights of the past year include the

structure determination of DNA-binding domains of GAL4 (both by NMR and X-ray crystallography) and of c-Myb, a protein related to the helix-turn-helix family of proteins. Progress has also been made for other classes of DNA-binding protein, most notably for the TFIIIA-like zinc fingers, for which the architectural rules are now well understood.

L42 ANSWER 17 OF 24 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1992:531722 SCISEARCH Full-text
THE GENUINE ARTICLE: JL899
TITLE: TRANSCRIPTION REGULATION BY STEROID-HORMONES - A
COMPUTER-SIMULATION STUDY
AUTHOR: KOTHEKAR V (Reprint)
CORPORATE SOURCE: ALL INDIA INST MED SCI, DEPT BIOPHYS, NEW DELHI 110029,
INDIA (Reprint)
COUNTRY OF AUTHOR: INDIA
SOURCE: JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, (AUG 1992)
Vol. 10, No. 1, pp. 49-62.
ISSN: 0739-1102.
PUBLISHER: ADENINE PRESS INC, PO BOX 355/340, GUILDERLAND, NY 12084.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 39
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Three-dimensional structures of complexes of 66 amino acid-DNA binding domains of human progesterone (hPR), estrogen (hER) and glucocorticoid (hGR) receptors (proteins), with ten base pair DNA duplexes: d(AGGTCATGCT) . d(AGCATGACCT) and d(AGAACATGCT) . (AGCATGTTCT) were obtained using computer modeling and molecular mechanics techniques. Cartesian coordinates for the proteins were obtained from: 1) structural data of hER and hGR by NMR spectroscopy; 2) steric constraints imposed by tetrahedral coordination of the zinc ion to Cys residues, and 3) energy minimization in torsional and cartesian space. The proteins were made to interact with DNA (in B-form) in major groove through alpha-helical linker between the two zinc fingers. The geometry of the complexes was obtained by allowing them to slide, glide, penetrate in to and out of the groove, and to rotate about the helical axis. The complexes were energy minimized. Also maximized was the number of H-bonds between proteins and DNA. The complex structures were refined by molecular mechanics using AMBER 3.0. Structural parameters of DNA were analyzed in each complex and compared with those of native DNA optimized separately. The stereochemical differences of the complexes are discussed.

L42 ANSWER 18 OF 24 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1992:386270 SCISEARCH Full-text
THE GENUINE ARTICLE: HZ964
TITLE: STRUCTURAL REQUIREMENTS FOR HIGH-AFFINITY LIGAND-BINDING
BY ESTROGEN-RECEPTORS - A COMPARATIVE-ANALYSIS OF
TRUNCATED AND FULL LENGTH ESTROGEN-RECEPTORS EXPRESSED IN
BACTERIA, YEAST, AND MAMMALIAN-CELLS
AUTHOR: WOOGIE C H (Reprint); NILSSON G M; HEIERSON A; MCDONNELL D
P; KATZENELLENBOGEN B S
CORPORATE SOURCE: UNIV ILLINOIS, DEPT PHYSIOL & BIOPHYS, 524 BURRILL HALL,
407 S GOODWIN AVE, URBANA, IL 61801; UNIV ILLINOIS, COLL
MED, URBANA, IL 61801; KARO BIO AB, HUDDINGE, SWEDEN;
BAYLOR COLL MED, DEPT CELL BIOL, HOUSTON, TX 77030
COUNTRY OF AUTHOR: USA; SWEDEN
SOURCE: MOLECULAR ENDOCRINOLOGY, (JUN 1992) Vol. 6, No. 6, pp.
861-869.
ISSN: 0888-8809.
PUBLISHER: ENDOCRINE SOC, 4350 EAST WEST HIGHWAY SUITE 500, BETHESDA,
MD 20814-4110.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 33
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB In order to better understand the structural requirements for effective high affinity binding of estrogens and antiestrogens by the human estrogen receptor (ER); a comparative study was undertaken in which we examined: 1) native ER from the MCF-7 ER-positive human breast cancer cell line; 2) full length ER expressed in yeast; 3) the ER hormone binding

domain (amino acid residues 302-595) expressed in yeast; 4) a bacterially expressed protein A fusion product encoding a truncated ER (amino acid residues 240-595); and 5) a synthetic peptide encompassing amino acids 510-551 of the ER. The binding parameters studied included affinity, kinetics, structural specificity for ligands, and stability. Full length ER expressed in yeast was very similar to the MCF-7 ER in its affinity [dissociation constant (K(d)), 0.35 +/- 0.05 nM], dissociation rate (t1/2, 3-4 h at 25 C), and structural specificity for both reversible and covalently attaching affinity ligands. While the truncated ER expressed in yeast was similar to MCF-7 ER in its specificity of ligand binding, it showed a slightly reduced affinity for estradiol (K(d), 1.00 +/- 0.17 nM). The bacterially expressed ER also had a lower affinity for estradiol (K(d), 1.49 +/- 0.16 nM), which may be due in part to an increase in the dissociation rate (t1/2, 0.5 h at 25 C). The attachment of covalent affinity ligands and structural specificity for a variety of reversible ligands was comparable in the bacterially expressed ER to that observed for the receptors expressed in MCF-7 cells and yeast. Full length and truncated receptors expressed in yeast, as well as the bacterially expressed ER, were as stable as the full length MCF-7 ER, with minimal loss of the initial binding capacity of the unoccupied receptor even after 10 h at 25 C. In contrast, there was no binding of either reversibly (estradiol) or covalently attaching (ketononestrol aziridine, tamoxifen aziridine) ligands to a 42-amino acid synthetic peptide (human ER amino acids 510-551) comprising a portion of the hormone binding domain considered essential for ligand binding and which encompasses Cys-530, shown previously to be the amino acid covalently labeled with ER affinity labeling ligands. These studies demonstrate that the hormone binding domain of the ER alone (amino acids 302-595) is sufficient to bind ligand with good affinity (ca. 30% that of full length ER) and with appropriate ligand structural specificity. Such expressed truncated proteins should be valuable in further studies to characterize the three-dimensional structure of the ligand binding pocket of the receptor.

L42 ANSWER 19 OF 24 LIFESCI COPYRIGHT 2006 CSA on STN

ACCESSION NUMBER: 91:8023 LIFESCI Full-text

TITLE: Zinc fingers.

AUTHOR: Kaptein, R.

CORPORATE SOURCE: Bijvoet Cent. Biomol. Res., Univ. Utrecht, Utrecht, Netherlands

SOURCE: CURR. OPIN. STRUCT. BIOL., (1991) vol. 1, no. 1, pp. 63-70.

DOCUMENT TYPE: Journal

TREATMENT CODE: General Review

FILE SEGMENT: L

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Within the past year, the first three-dimensional structures of zinc-finger domains have become available. Using two-dimensional NMR methods, the solution conformations have been determined for three classes of zinc-finger peptides: the single-finger domains of the yeast transcriptional activators ADR1 and SW15 and of the *Xenopus* protein Xfin, which are all homologous with the prototypal fingers of the transcription factor TFIIIA (CC/HH zinc fingers); the metal-binding site of a retroviral protein derived from the gag gene (CC/HC zinc finger); and the DNA-binding domain of the glucocorticoid receptor, a member of the superfamily of steroid/thyroid hormone receptors (two CC/CC zinc fingers).

L42 ANSWER 20 OF 24 LIFESCI COPYRIGHT 2006 CSA on STN

ACCESSION NUMBER: 90:61904 LIFESCI Full-text

TITLE: Solution structure of the glucocorticoid receptor DNA-binding domain.

AUTHOR: Haerd, T.; Kellenbach, E.; Boelens, R.; Maler, B.A.; Dahlman, K.; Freedman, L.P.; Carlstedt-Duke, J.; Yamamoto, K.R.; Gustafsson, J.; Kaptein, R.

CORPORATE SOURCE: Dep. Chem., Univ. Utrecht, Padualaan 8, 3584 CH Utrecht, Netherlands

SOURCE: SCIENCE (WASH.), (1990) vol. 249, no. 4965, pp. 157-160.

DOCUMENT TYPE: Journal

FILE SEGMENT: N; N3

LANGUAGE: English

SUMMARY LANGUAGE: English

AB The three-dimensional structure of the DNA-binding domain (DBD) of the glucocorticoid receptor has been determined by nuclear magnetic resonance spectroscopy and distance geometry. The structure of a 71-residue protein fragment containing two "zinc finger" domains is based on a large set of proton-proton distances derived from nuclear Overhauser enhancement spectra, hydrogen bonds in previously identified secondary structure elements, and coordination of two zinc atoms by conserved cysteine residues. The DBD is found to consist of a globular body from which the finger regions extend. A model of the dimeric complex between the DBD and the glucocorticoid response element is proposed.

L42 ANSWER 21 OF 24 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on

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ACCESSION NUMBER: 1995:124720 BIOSIS Full-text
DOCUMENT NUMBER: PREV199598139020
TITLE: DNA recognition by the oestrogen receptor: From solution to the crystal.
AUTHOR(S): Schwabe, John W. R. [Reprint author]; Chapman, Lynda; Finch, John T.; Rhodes, Daniela; Neuhaus, David
CORPORATE SOURCE: MRC Lab. Molecular Biol., Hills Road, Cambridge CB2 2QH, UK
SOURCE: Structure (London), (1993) Vol. 1, No. 3, pp. 187-204.
ISSN: 0969-2126.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 29 Mar 1995
Last Updated on STN: 29 Mar 1995

AB Background: The steroid/nuclear hormone receptors are a large family of conserved ligand-activated transcription factors that regulate gene expression through binding to response elements upstream of their target genes. Most members of this family bind to DNA as homodimers or heterodimers and recognize the sequence, spacing and orientation of the two half-sites of their response elements. The recognition and discrimination of the sequence and arrangements of these half-sites are mediated primarily by a highly conserved DNA-binding domain. Results: Here we describe the DNA-binding properties of the isolated DNA-binding domain of the oestrogen receptor, the ERDBD, and its refined NMR structure. This domain is monomeric in solution, but two molecules bind cooperatively to specific DNA sequences; this cooperativity determines the arrangement of half-sites that is recognized by the ERDBD. The 10 carboxy-terminal residues and a region of 15 residues within the domain are disordered in the solution structure, yet are important for DNA binding. Conclusion: The cooperative nature of ERDBD binding to DNA is important. The previously-determined X-ray structure of the ERDBD dimer bound to DNA shows that the 15 internal residues disordered in solution make contact both with DNA and with the corresponding region of the other monomer. These results suggest that these residues become ordered during the process of binding to DNA, forming the dimer interface and thus contributing to the cooperative interaction between monomers.

L42 ANSWER 22 OF 24 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
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ACCESSION NUMBER: 1995:63380 BIOSIS Full-text
DOCUMENT NUMBER: PREV199598077680
TITLE: Molecular dynamics simulations in solvent of the glucocorticoid receptor protein in complex with a glucocorticoid response element DNA sequence.
AUTHOR(S): Harris, Lester F.; Sullivan, Michael R.; Popken-Harris, Pamela D.; Hickok, David F.
CORPORATE SOURCE: Abbott Northwestern Hosp. Cancer Res. Lab., 800 E. 28th St., Minneapolis, MN 55407, USA
SOURCE: Journal of Biomolecular Structure and Dynamics, (1994) Vol. 12, No. 2, pp. 249-270.
CODEN: JBSDD6. ISSN: 0739-1102.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 8 Feb 1995
Last Updated on STN: 8 Feb 1995

AB We investigated protein/DNA interactions, using molecular dynamics simulations computed in solvent between the glucocorticoid receptor (GR) DNA binding domain (DBD) amino acids and DNA of a glucocorticoid receptor response element (GRE). We compared findings obtained from a fully solvated 80 Angstrom water droplet GR DBD/GRE model with those from a 10 Angstrom water layer GR DBD/GRE model. Hydrogen bonding interactions were monitored. In addition, van der Waals and electrostatic interaction energies were calculated. Molecular dynamics simulations from both models yielded similar findings, amino acids of the GR DBD DNA recognition helix formed both direct and water mediated hydrogen bonds at cognate codon/anticodon nucleotide base sites within the GRE right major groove halfsite. Likewise GR DBD amino acids in a beta strand structure adjacent to the DNA recognition helix formed both direct and water mediated hydrogen bonds at cognate codon/anticodon nucleotide base and backbone sites. We also investigated protein/ DNA interactions with a 10 Angstrom water layer model consisting of the same GR DBD as above but with a predicted alpha helix attached to the carboxyl terminus of the GR DBD docked at the same GRE as above with additional flanking nucleotides. In this model, the interactions between amino acids of the DNA recognition helix and beta strand and nucleotides within the GRE right major groove halfsite were at cognate codon/anticodon nucleotide sites as found in the two models above. In addition, amino acids within the predicted alpha helix located on the carboxyl terminus of the GR DBD interacted at codon/anticodon nucleotide sites on the DNA backbone of the GRE flanking nucleotides. These interactions together induced breakage of Watson-Crick nucleotide base pairing hydrogen bonds, resulting in bending of the DNA. strand elongation and unwinding events similar to those described for helicases.

L42 ANSWER 23 OF 24 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
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ACCESSION NUMBER: 1993:315989 BIOSIS Full-text
DOCUMENT NUMBER: PREV199396024339
TITLE: Synthesis of several new isoxazole, imidazo(1,2-a)pyridine,
imidazo(1,2-a)pyrimidine, benzoxadiazine and benzothiazine
derivatives from hydroximoyl halides.
AUTHOR(S): Abdelhamid, Abdou O. [Reprint author]; Abdou, Sadek E.;
Mahgoub, Sayed A.
CORPORATE SOURCE: Dep. Science, King Khalid Military Academy, P.O. Box 22140,
Riyadh 11495, Saudi Arabia
SOURCE: Archives of Pharmacal Research (Seoul), (1992) Vol. 15, No.
4, pp. 317-321.
CODEN: APHRDQ. ISSN: 0253-6269.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 12 Jul 1993
Last Updated on STN: 3 Jan 1995

AB Furoylhydroximoyl chloride 3 reacted with 2-aminopyridine, 2-aminopyrimidine, O-aminophenol, O-phenylenediamine and aminothiophenol to afford imidazo(1,2-a)pyridine 6, imidazo(1,2-a)pyrimidine 8, benzoxadiazine 10, nitrosobenzopyrazine 13a and nitrosobenzothiazine 13b, respectively. Isoxazoline 18 and pyrrolidino(3,4-d)isoxazolin-4,6-dione derivatives 19a and 19b obtained by the reaction of 3 with acrylonitrile and N-arylmaleimide. Hydroximoyl chloride 3 reacted with thiophenol and sodium benzene-sulfinate to yield furylglyoxaloxime 16a and 16b, respectively. Hydroximoyl chloride 3 reacted also with some active methylene compound to give isoxazole derivatives 20-23, respectively.

L42 ANSWER 24 OF 24 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
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ACCESSION NUMBER: 1990:514948 BIOSIS Full-text
DOCUMENT NUMBER: PREV199090132224; BA90:132224
TITLE: PROTON NMR STUDIES OF THE GLUCOCORTICOID
RECEPTOR DNA-BINDING DOMAIN SEQUENTIAL ASSIGNMENTS
AND IDENTIFICATION OF SECONDARY STRUCTURE ELEMENTS.
AUTHOR(S): HARD T [Reprint author]; KELLENBACH E; BOELENS R; KAPTEIN
R; DAHLMAN K; CARLSTEDT-DUKE J; FREEDMAN L P; MALER B A;
HYDE E I; ET AL
CORPORATE SOURCE: CELL BIOL GENETICS PROGRAM, MEMORIAL SLOAN-KETTERING
CENTER, NEW YORK, NY 10023, USA
SOURCE: Biochemistry, (1990) Vol. 29, No. 38, pp. 9015-9023.
CODEN: BICHAW. ISSN: 0006-2960.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 19 Nov 1990
Last Updated on STN: 19 Nov 1990

AB Two protein fragments containing the DNA-binding domain (DBD) of the glucocorticoid receptor (GR) have been studied by two-dimensional 1H NMR spectroscopy. The two peptides (93 and 115 residues, respectively) contain a common segment corresponding to residues C440-I519 of the rat GR or residues C421-I500 of the human GR and include two Zn-binding "finger" domains. The structures of this segment are almost identical in the two protein fragments, as judged from chemical shifts and sequential NOE connectivities. More than 90% of all observable 1H resonances within a 71-residue segment encompassing C440-R510 (rat GR) could be sequentially assigned by standard techniques, and stereospecific assignments could be made for the methyl groups in four valine residues within this segment. Sequential NOE connectivities indicate several elements of secondary structure including two α -helical segments consisting of residues S459-E469 and P493-G504, a type I reverse turn between residues R479 and C482, a type II reverse turn between residues L475 and G478, and several regions of extended peptide conformation. No evidence for α -helical conformation was found within the two putative zinc-finger domains, indicating that the structures of these domains differ from that of TFIIIA-type zinc fingers. The observation of some very slowly exchanging amide protons in the N-terminal (CI) domain of the DBD in combination with slow rotation of the Y452 aromatic ring indicates that this domain has a restricted conformational flexibility compared to the C-terminal (CII) domain. We also observe several long-range NOE connectivities within C440-R510, suggesting that the sequential assignments presented here will provide a basis for a complete structure determination of this segment of the GR.

=> s 17 and ligand binding domain

TOTAL FOR ALL FILES

L49 404 L7 AND LIGAND BINDING DOMAIN

=> s l49 and (site II or site 2 or site-II or site-2)
TOTAL FOR ALL FILES
L56 1 L49 AND (SITE II OR SITE 2 OR SITE-II OR SITE-2)

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L56 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:80449 CAPLUS Full-text
DOCUMENT NUMBER: 140:157927
TITLE: Homology modeling of nuclear hormone receptor
Site II and design of Site
II ligands
INVENTOR(S): Dowsyko, Arthur; Nadler, Steven G.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 276 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009016	A2	20040129	WO 2003-US22299	20030717
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,				
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,				
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,				
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,				
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,				
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1575502	A2	20050921	EP 2003-765637	20030717
EP 1575502	A3	20051123		
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006223110	A1	20061005	US 2003-621807	20030717
PRIORITY APPLN. INFO.:			US 2002-396907P	P 20020718
			WO 2003-US22299	W 20030717

AB A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.

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